TOXIC SUBSTANCES CONTROL ACT (TSCA)

PL 94-469

CANDIDATE LIST OF CHEMICAL SUBSTANCES

ADDENDUM III

Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials

March 1978

U.S. Environmental Protection Agency
Office of Toxic Substances
Washington, DC 20460

TABLE OF CONTENTS

INTRODUCTION

The Toxic Substances Control Act (TSCA), Public Law 94-469, requires the U.S. Environmental Protection Agency to compile, keep current, and publish a list of each chemical substance which is manufactured, imported, or processed in the United States for commercial purposes. Under the authority of Section 8 of TSCA, EPA will compile this inventory from reports prepared and submitted by manufacturers, importers, and processors of chemical substances in accordance with Inventory Reporting Regulations (40 CFR 710). These regulations were published in the FEDERAL REGISTER on December 23, 1977 (pages 64572 to 64596), and became effective on January 1, 1978.

In April 1977, EPA published the TSCA Candidate List of Chemical Substances, which identifies over 30,000 chemical substances. The Candidate List was prepared to assist persons in reporting chemical substances for the Inventory. In January 1978, EPA published two addenda to the Candidate List, the first identifying petroleum refinery intermediate and final process stream chemical substances, and the second identifying an additional 3,000 Class 1 chemical substances. A Class 1 chemical substance is one whose composition can be represented by a definite chemical structure diagram.

This document, addendum III to the Candidate List, identifies primarily Class 2 chemical substances, and provides a mechanism for identifying and reporting others. A Class 2 chemical substance is one whose composition cannot be represented by a definite chemical structure diagram. Some chemical substances identified in this addendum are defined, in part, in terms of the processes by which they are manufactured. Other chemical substances are simply identified by names which are widely recognized and need no further definition.

Certain common materials of commerce, such as inorganic glasses, are defined by the Inventory Reporting Regulations as mixtures. To facilitate reporting, this addendum defines certain categories which encompass the individual chemical substances manufactured in the production of these mixtures.

This addendum is organized into ten sections, listing terms developed by EPA in cooperation with various trade associations and other agents. They represent industries involved in the manufacture of Class 2 chemical substances which are difficult to define, either due to slight variations of process or because the composition of these substances is not completely known or is variable. Although this addendum identifies chemical substances which are common to specific industries, it does not include all reportable chemical substances manufactured within these industries. Furthermore, any persons who manufacture such substances may use the nomenclature presented in this addendum to report for the Inventory if this nomenclature accurately describes the chemical substances they manufacture.

All chemical substances identified in this addendum, with the exception of those in Section I (multi-component Class 2 substances derived from natural fats and oils or synthetic substitutes), are listed with CAS Registry Numbers and EPA Code Designations, and may be reported on Form A. The substances identified in Section I must be reported on Form C according to the procedures outlined in that section.

Section I

CLASS 2 CHEMICAL SUBSTANCES DERIVED FROM NATURAL FATS AND OILS AND SYNTHETIC SUBSTITUTES

An Alternate Procedure for Substance Identification and Reporting for the Chemical Substance Inventory

General

This section presents an alternate and relatively simple procedure for identifying and reporting certain multicomponent Class 2 chemical substances derived from natural fats and oils and synthetic long-chain alkyl substitutes. The procedure was developed by The Soap and Detergent Association in conjunction with the EPA and is intended to standardize the identification of substances manufactured and used extensively in the soap and detergent industry. This standardization should provide for easier and more certain reporting and recording of information for these substances. Accordingly, the procedure may be used to report multicomponent soaps and surface active agents (and also their precursors and derivatives) manufactured, imported, or processed for such uses as wetting agents, emulsifiers, dispersants, and penetrants. Its applicability, however, should extend beyond the soap and detergent industry.

This procedure may not be used to report any single component Class 1 chemical substance (i.e., a substance whose composition may be represented by a definite chemical structure diagram) or any combination of such substances prepared by mixing without chemical reaction. Furthermore, it should not be used in those cases where the person reporting considers its applicability to be marginal or in question. Instead, the conventional procedures should be followed for chemical substance identification and reporting, as specified in the EPA publication "Reporting for the Chemical Substance Inventory" (December 1977).

The Class 2 chemical substances which may be reported following procedures specified here are complex, multicomponent materials whose individual components have a common structural feature: one or more long-chain alkyl groups to which is attached a chemically functional group or groups. These components differ from one another with respect to one or more of the following long-chain alkyl group characteristics: length (carbon number), saturation, structure (linear or branched), and/or the position of functional group attachment(s).

Before 1950, most of these substances were derived commercially from natural sources. However, synthetically-derived sources of similar composition have since been developed and are presently used interchangeably with natural sources.

Substance Identification

According to procedures specified in this section, certain of these Class 2 chemical substances may be identified by systematically-derived, chemically-descriptive SDA Substance Names. The proper SDA Substance Name for each is that which most precisely describes the chemical composition of the substance. Each substance is reported on Inventory Report Form C and identified only by the SDA Substance Name and special SDA Reporting Number, and not in terms of source, blend, process, or reaction information. During form processing, each substance reported following this procedure will be assigned a CAS Registry Number which will appear on the Inventory with the SDA Substance Name and Reporting Number and with substance synonyms, if reported.

SDA Substance Names consist of two or, in some cases, three parts. The two parts common to all SDA Substance Names are: (1) the Alkyl Descriptor, A, which describes the long-chain alkyl groups of the substance, and (2) the Functionality Descriptor, F, which identifies the functional group(s) of the substance. A third part, the Salt Descriptor, S, identifies the cation(s) of any salt.

SDA Substance Names are systematically constructed according to the following formats:

(A) alkyl (F),

or in the case of salts,

(A) alkyl (F)(S),

where A denotes the Alkyl Descriptor; F, the Functionality Descriptor; and S, the Salt Descriptor.

For example, the SDA Substance Name for a fatty amine which contains predominantly C_{10}-C_{16} saturated alkyl chain-lengths is:

C_{10}-C_{16} alkyl amine

where the phrase "C_{10}-C_{16}" corresponds to the Alkyl Descriptor (A), and "amine", to the Functionality Descriptor (F).

Similarly, the SDA Substance Name for the sodium salt of a fatty carboxylic acid comprised predominantly of C_{18} saturated and C_{18} unsaturated alkyl chains is:

C_{18} and C_{18} unsaturated alkyl carboxylic acid sodium salt

where the phrase "C_{18} and C_{18} unsaturated" corresponds to the Alkyl Descriptor (A); "carboxylic acid", to the Functionality Descriptor (F); and "sodium salt", to the Salt Descriptor (S).

The Class 2 chemical substances covered by this section are limited to those whose composition may be described using the Alkyl, Functionality, and Salt Descriptors listed in Tables 1, 2, and 3, respectively. These descriptors, discussed in detail below, may be combined in the SDA Substance Name format to describe more than 5,000 multicomponent Class 2 chemical substances.

Alkyl Description

Table 1 lists the Alkyl Descriptors covered by this system of substance identification; assigned to each is a two-digit Alkyl Descriptor Code used in generating the SDA Reporting Numbers, described later. Each Descriptor identifies a distribution of alkyl groups in terms of carbon chainlength, saturation and/or unsaturation, and linear or branched structure. Alkyl group distributions are inclusive of both even and odd alkyl chainlengths.

The Descriptors of Table 1 were chosen to cover the predominant long-chain alkyl group distributions actually present in most commercial multicomponent Class 2 substances of this type, and to provide for each as precise a description as practical. Use of this procedure is predicated on selecting the narrowest alkyl distribution (Alkyl Descriptor) which describes the predominant long-chain alkyl groups of the substance reported. In this context, the term "predominant" means that about 80 to 100 percent of all long-chain alkyl groups are included within the description.

In the Alkyl Descriptor, a saturated, linear long-chain alkyl group is denoted by "C_x" where the subscript x indicates the number of carbon atoms in the alkyl chain. Unsaturated and multiple branched alkyl groups are denoted by "C_x unsaturated" and "C_x branched", respectively.

By convention, the number of carbon atoms in a long-chain alkyl group includes all long-chain alkyl and functional group carbon atoms, other than those contained in an aromatic ring, which are connected to each other in a unbroken chain of carbon-carbon bonds. For example, the alkyl chainlength, designated by "R" in the representative structural diagrams found in Table 2, includes the acyl carbon of carboxylic acids and their derivatives, and the total number of carbon atoms in such structures as $R\text{-}CH_2\text{-}OH$ or $R\text{-}CH{=}CH_2$. The alkyl group does not include, however, functional group carbon atoms which are part of a phenyl ring, or are separated from the alkyl chain by a phenyl group or an atom other than carbon, e.g., R-  , $R\text{-}N(CH_3)_2$, or $R\text{-}O(CH_2)_3NH_2$.

Unless specified otherwise, the alkyl groups identified by each Alkyl Descriptor are linear, or essentially linear, hydrocarbon chains. The natural fats and oils listed below provide such alkyl groups:

Vegetable		Animal	Marine
Avocado	Peanut	Grease	Herring
Babassu	Rapeseed	Lard	Menhaden
Castor	Rice Bran	Neatsfoot	Salmon
Coconut	Safflower	Poultry	Sardine
Corn	Safflower (high oleic)	Tallow	Sperm Body (whale)
Cottonseed	Sesame		Sperm Head (whale)
Crambe	Sorghum		Whale
Linseed	Soybean		
Olive	Sunflower		
Oiticica	Tung		
Palm	Wheat Germ		
Palm-kernel			

These sources provide both saturated and unsaturated alkyl groups; castor oil provides a C_{18} hydroxy substituted alkyl group. Alkyl groups derived from other natural sources are not covered by this procedure.

Synthetic sources can provide linear or essentially linear alkyl groups, i.e., chain branching, if any, is limited to no more than one secondary methyl (CH_3-) or ethyl (C_2H_5-) group per alkyl chain. For purposes of this section, the latter type of alkyl chain is included within the designation "linear". Multiple branched alkyl groups, derived exclusively from synthetic sources, have separate Alkyl Descriptors.

Some Class 2 chemical substances covered by this procedure are comprised of components which have two or more long-chain alkyl groups, e.g., (dialkyl) amine, or (dialkyl) dimethyl ammonium chloride. This procedure may be used to identity such substances provided that each long-chain alkyl group is describable, in its predominant composition, by an Alkyl Descriptor found in Table 1 and that none of these long-chain alkyl groups is a single component structure describable by a definite chemical structural diagram.